wwPDB X-ray Structure Validation Summary Report (i)

Apr 14, 2025 – 05:01 PM JST

PDB ID	:	8KAH / pdb_00008kah
Title	:	Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 18nt target DNA
Authors	:	Chen, Y.; Chen, J.; Liu, L.
Deposited on	:	2023-08-03
Resolution	:	3.36 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

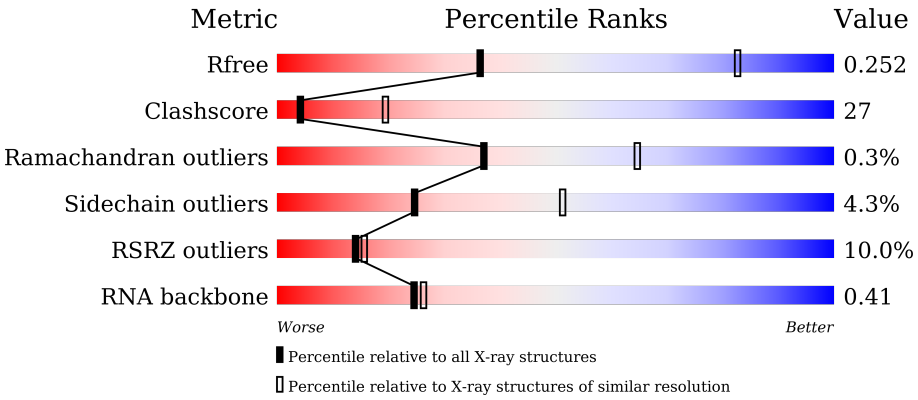
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1012 (3.40-3.32)
Clashscore	180529	1035 (3.40-3.32)
Ramachandran outliers	177936	1037 (3.40-3.32)
Sidechain outliers	177891	1037 (3.40-3.32)
RSRZ outliers	164620	1012 (3.40-3.32)
RNA backbone	3690	1010 (3.74-2.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	34	15% 41% 32% 12%
1	E	34	3% 12% 41% 38% • 6%
2	B	1368	7% 53% 42% • •
2	F	1368	14% 50% 43% • •

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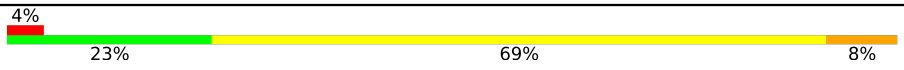
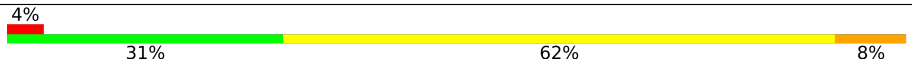
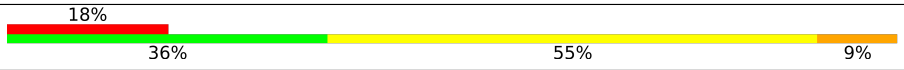
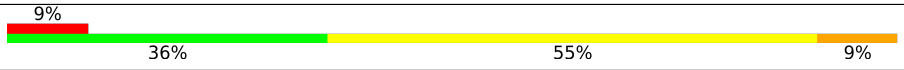
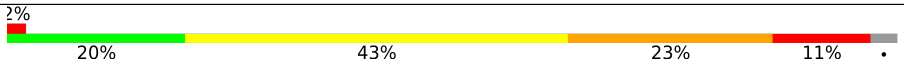
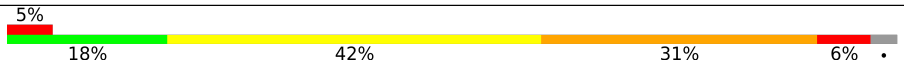
Mol	Chain	Length	Quality of chain
3	C	26	
3	G	26	
4	D	11	
4	H	11	
5	I	65	
5	J	65	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27025 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	34	Total	C	N	O	P	0	0	0
			725	325	127	239	34			
1	E	32	Total	C	N	O	P	0	0	0
			685	307	123	223	32			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1322	Total	C	N	O	S	0	0	0
			10732	6827	1864	2019	22			
2	F	1327	Total	C	N	O	S	0	0	0
			10695	6814	1845	2014	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
F	10	ALA	ASP	engineered mutation	UNP Q99ZW2
F	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	P	0	0	0
			521	254	85	157	25			
3	G	26	Total	C	N	O	P	0	0	0
			521	254	85	157	25			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			
4	H	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			

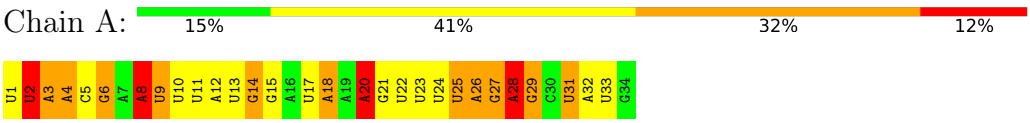
- Molecule 5 is a RNA chain called RNA (65-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	63	Total	C	N	O	P	0	0	0
			1348	603	245	437	63			
5	J	63	Total	C	N	O	P	0	0	0
			1348	603	245	437	63			

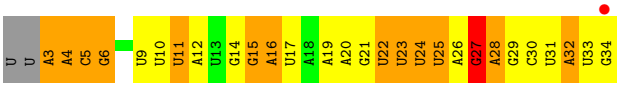
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

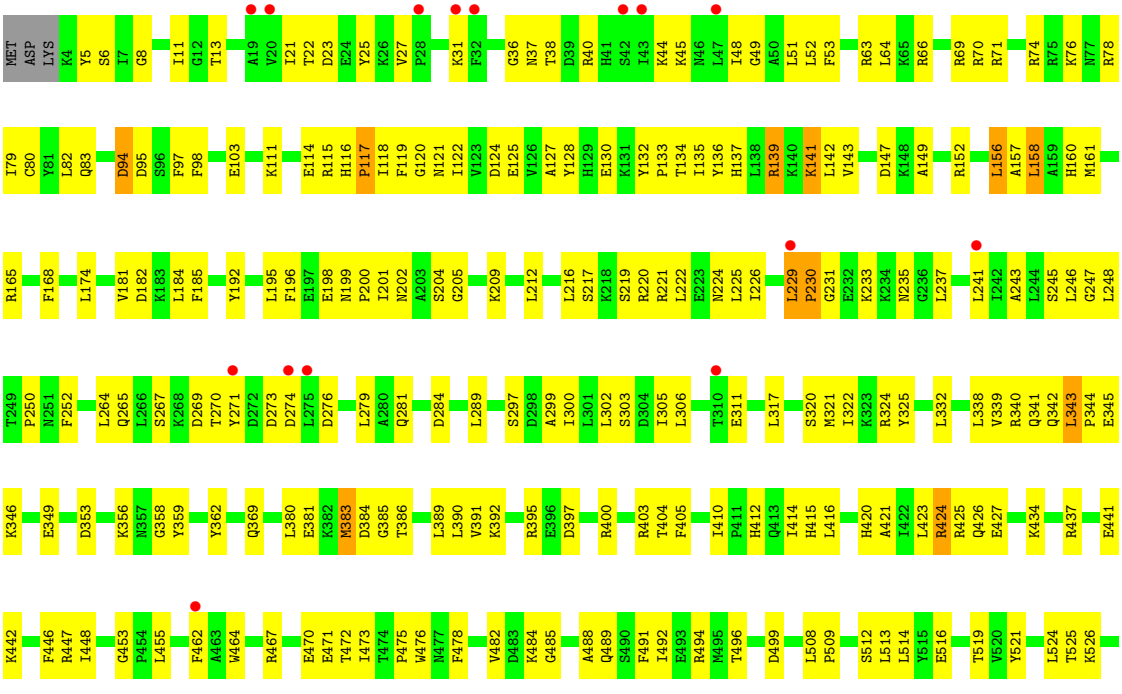
• Molecule 1: RNA (34-MER)

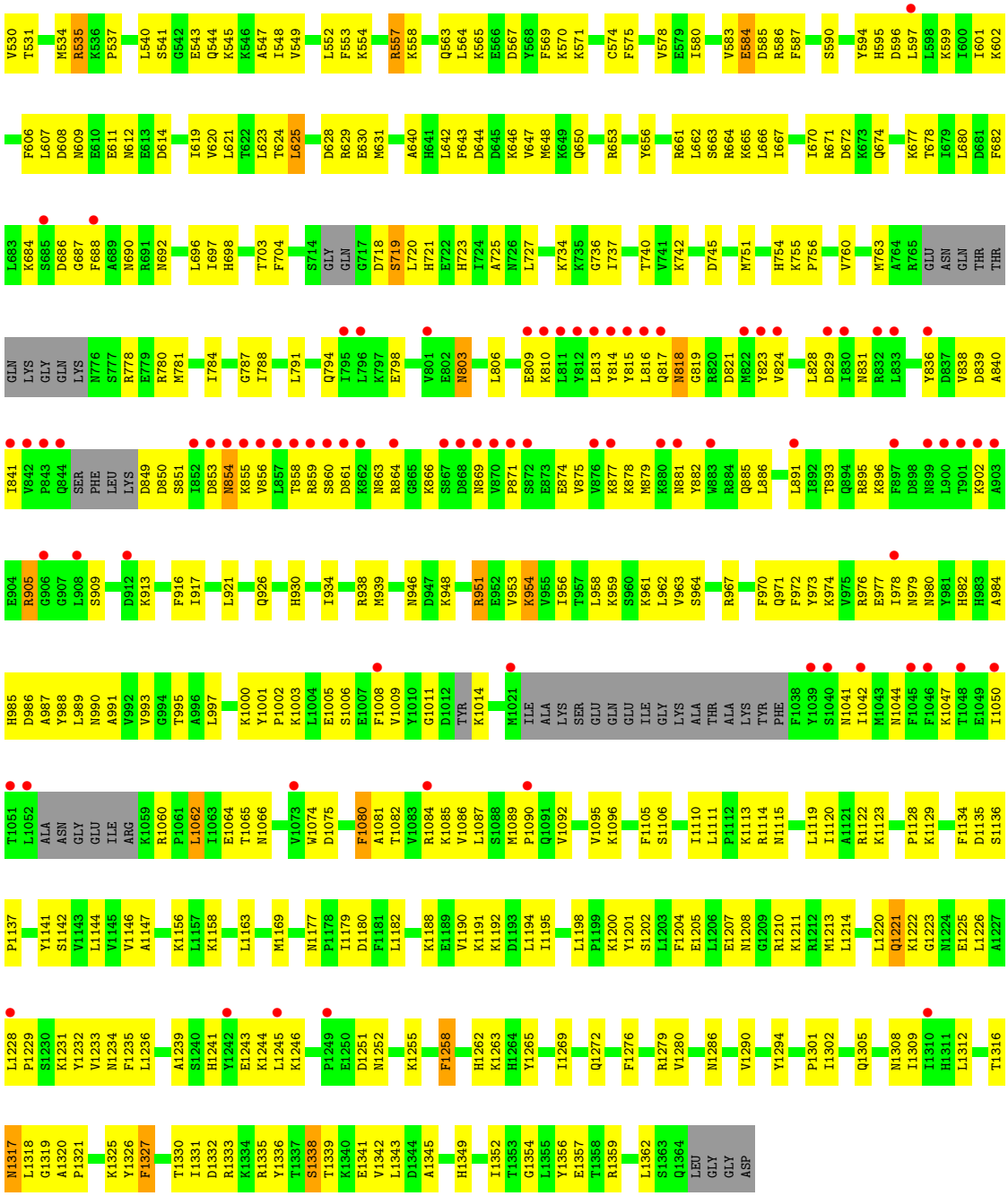


• Molecule 1: RNA (34-MER)

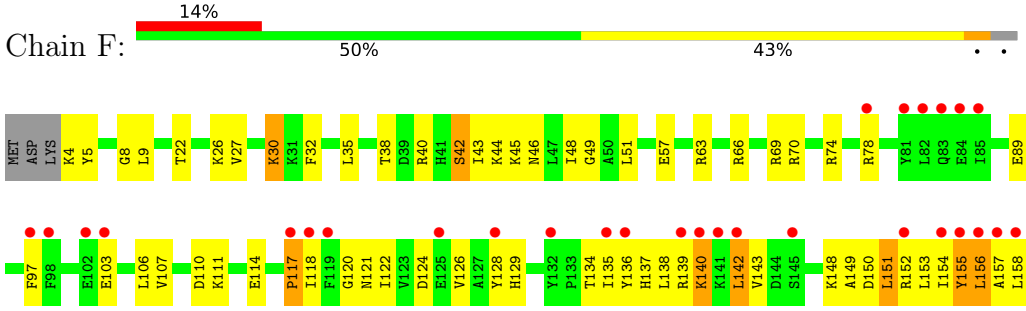


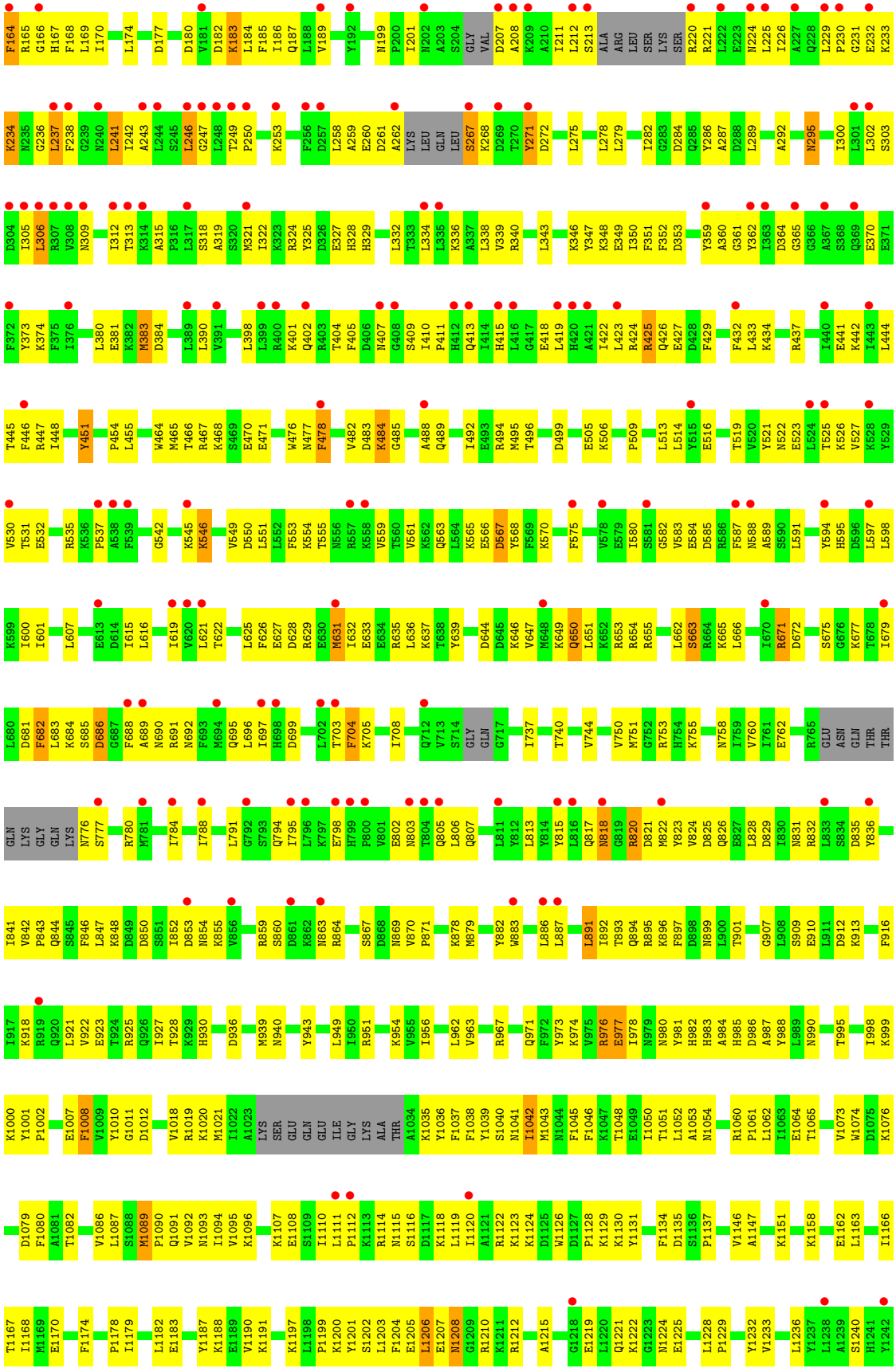
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

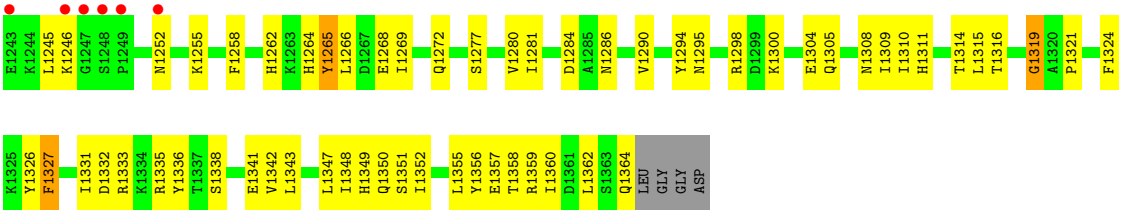




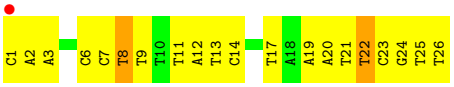
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



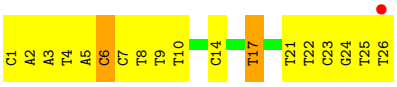

F164 R165 G166 H167 F168 L169 I170 L174 D177 D180 V181 D182 K183 L184 F185 I186 Q187 L188 V189 Y192 N199 P200 I201 N202 A203 S204 GLY VAL D207 A208 K209 A210 I211 L212 S213 ALA ARG LEU SER LYS SER R220 R221 L222 E223 N224 L225 I226 A227 Q228 L229 P230 G231 E232 K233
K234 N235 G236 L237 F238 G239 N240 L241 I242 A243 L244 S245 L246 G247 L248 T249 P250 K253 F255 D257 L258 A259 E260 D261 A262 LYS LEU GLN LEU S267 K268 D269 T270 Y271 D272 L275 L278 L279 I282 G283 D284 Q285 Y286 A287 D288 L289 A292 N295 I300 L301 L302 S303
D304 I305 L306 R307 V308 N309 I312 T313 K314 A315 P316 L317 S318 A319 S320 M321 I322 K323 R324 Y325 D326 E327 H328 H329 L332 T333 L334 L335 K336 A337 L338 V339 R340 L343 K346 Y347 K348 E349 I350 F351 F352 D353 Y359 A360 G361 Y362 I363 D364 G365 G366 A367 S368 Q369 E370 E371
F372 Y373 K374 F375 I376 L380 E381 K382 M383 D384 L389 L390 V391 L398 L399 R400 K401 Q402 R403 T404 F405 D406 N407 G408 S409 I410 P411 H412 Q413 I414 H415 L416 G417 E418 L419 H420 A421 I422 L423 R424 R425 Q426 E427 D428 F429 F432 L433 K434 R437 I440 E441 K442 L443 L444
T445 F446 R447 I448 Y451 P454 L455 W464 M465 T466 R467 K468 S469 E470 E471 W476 N477 F478 V482 D483 K484 G485 A488 Q489 I492 E493 R494 M495 T496 D499 E505 K506 P509 L513 L514 Y515 E516 T519 V520 Y521 N522 E523 L524 T525 K526 V527 K528 Y529
V530 T531 E532 R535 K536 P537 A538 F539 G542 K545 K546 V549 D550 L551 L552 F553 K554 T555 N556 R557 K558 V559 T560 V561 K562 Q563 L564 K565 E566 D567 Y568 F569 K570 F575 V578 E579 I580 S581 G582 V583 E584 D585 K586 F587 N588 A589 S590 L591 Y594 H595 D596 L597 L598
K599 I600 I601 L607 E613 D614 I615 L616 I619 V620 L621 T622 L625 F626 E627 D628 R629 E630 M631 I632 E633 E634 R635 L636 K637 T638 Y639 D644 D645 K646 V647 M648 K649 Q650 L651 K652 R653 R654 R655 L662 S663 R664 K665 L666 I670 R671 D672 S675 G676 K677 T678 I679
L680 D681 F682 L683 K684 S685 D686 G687 F688 A689 N690 R691 N692 F693 M694 Q695 L696 I697 H698 D699 L702 T703 F704 K705 I708 Q712 V713 S714 GLY GLN G717 I737 T740 V744 V750 M751 G752 R753 H754 K755 N758 I759 V760 I761 E762 R765 GLU ASN GLN THR THR
GLN LYS GLY GLN LYS N776 S777 R780 M781 I784 I788 L791 G792 S793 Q794 I795 L796 K797 E798 H799 P800 V801 E802 N803 T804 Q805 L806 Q807 L811 Y812 L813 Y814 Y815 L816 Q817 N818 G819 R820 D821 M822 Y823 V824 D825 Q826 E827 L828 D829 I830 N831 R832 L833 S834 D835 Y836
I841 V842 P843 Q844 S845 F846 L847 K848 D849 D850 S851 I852 D853 N854 K855 V856 R859 S860 D861 K862 N863 R864 S867 D868 N869 V870 P871 K878 M879 Y882 W883 L886 L887 L891 I892 T893 Q894 R895 K896 F897 D898 N899 L900 T901 G907 L908 S909 E910 L911 D912 K913 F916
I917 K918 R919 Q920 L921 V922 E923 T924 R925 Q926 I927 T928 K929 H930 D936 M939 N940 Y943 L949 I950 R951 K954 V955 I956 L962 V963 R967 Q971 F972 Y973 K974 V975 R976 E977 I978 N979 N980 Y981 H982 H983 A984 H985 D986 A987 Y988 L989 N990 T995 I998 K999
K1000 Y1001 P1002 E1007 F1008 V1009 Y1010 G1011 D1012 Y1018 R1019 K1020 M1021 I1022 A1023 LYS SER GLU GLN GLU ILE GLY LYS ALA THR A1034 K1035 Y1036 F1037 F1038 Y1039 S1040 N1041 I1042 M1043 N1044 F1045 F1046 K1047 T1048 E1049 I1050 T1051 L1052 A1053 N1054 R1060 P1061 L1062 I1063 E1064 T1065 V1073 W1074 D1075 K1076
D1079 F1080 A1081 T1082 V1086 L1087 S1088 M1089 P1090 Q1091 V1092 N1093 I1094 V1095 K1096 K1107 E1108 S1109 I1110 L1111 P1112 K1113 R1114 N1115 S1116 D1117 K1118 I1119 I1120 A1121 R1122 K1123 K1124 D1125 W1126 D1127 P1128 K1129 K1130 Y1131 F1134 D1135 S1136 P1137 V1146 A1147 K1151 K1158 E1162 L1163 I1166
T1167 I1168 M1169 E1170 F1174 P1178 I1179 L1182 E1183 Y1187 K1188 E1189 V1190 K1191 K1197 L1198 P1199 K1200 Y1201 S1202 L1203 F1204 E1205 L1206 E1207 N1208 G1209 R1210 K1211 R1212 A1215 G1218 E1219 L1220 Q1221 K1222 G1223 N1224 E1225 L1228 P1229 Y1232 V1233 L1236 Y1237 L1238 A1239 S1240 H1241 Y1242



• Molecule 3: DNA (26-MER)



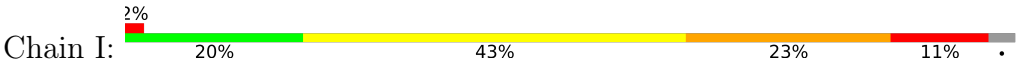
• Molecule 3: DNA (26-MER)

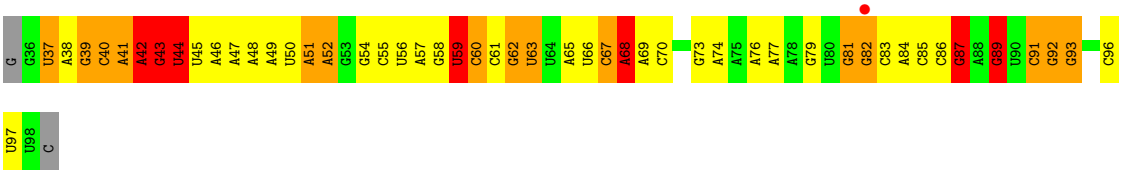


• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

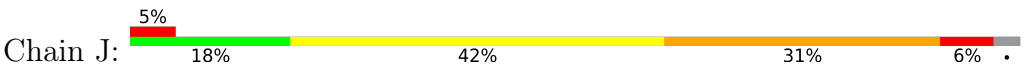
• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

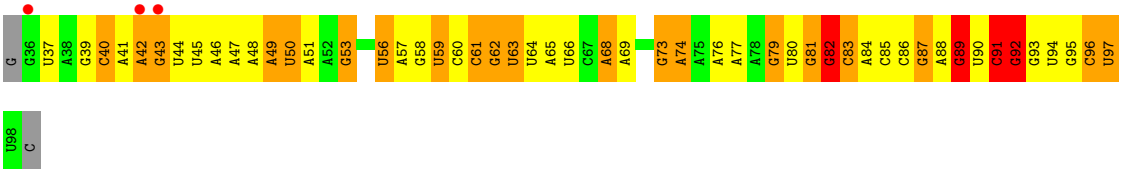
• Molecule 5: RNA (65-MER)





• Molecule 5: RNA (65-MER)




G
G36
U37
A38
G39
C40
A41
A42
G43
U44
U45
A46
A47
A48
A49
U50
A51
A52
G53
U56
A57
G58
U59
C60
C61
G62
U63
U64
A65
U66
C67
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G73
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A75
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A77
A78
G79
U80
G81
G82
C83
A84
C85
C86
G87
A88
G89
U90
C91
G92
G93
U94
G95
C96
U97
U98
C

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	145.21Å 130.60Å 148.73Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	48.23 – 3.36 48.23 – 3.36	Depositor EDS
% Data completeness (in resolution range)	59.4 (48.23-3.36) 73.8 (48.23-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.230 , 0.255 0.229 , 0.252	Depositor DCC
R_{free} test set	75003 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.069 for l,-k,h	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	27025	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.01	1/811 (0.1%)	1.81	32/1261 (2.5%)
1	E	0.87	0/767	1.73	23/1193 (1.9%)
2	B	0.58	1/10915 (0.0%)	0.80	11/14673 (0.1%)
2	F	0.58	2/10879 (0.0%)	0.78	4/14636 (0.0%)
3	C	1.42	6/581 (1.0%)	1.36	6/893 (0.7%)
3	G	1.25	1/581 (0.2%)	1.34	4/893 (0.4%)
4	D	1.51	1/251 (0.4%)	1.41	3/387 (0.8%)
4	H	1.49	1/251 (0.4%)	1.36	2/387 (0.5%)
5	I	1.03	1/1509 (0.1%)	1.90	61/2350 (2.6%)
5	J	0.93	0/1509	1.80	55/2350 (2.3%)
All	All	0.73	14/28054 (0.0%)	1.10	201/39023 (0.5%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	DA	C3'-O3'	-10.11	1.30	1.44
4	H	3	DT	C1'-N1	6.85	1.58	1.49
3	C	8	DT	C3'-O3'	-6.36	1.35	1.44
5	I	41	A	N9-C4	-6.20	1.34	1.37
2	F	1319	GLY	C-N	-5.73	1.20	1.34

The worst 5 of 201 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	91	C	C4-C5-C6	-9.82	112.49	117.40
5	J	76	A	C8-N9-C4	-9.81	101.88	105.80
3	C	14	DC	O4'-C4'-C3'	-9.62	100.23	106.00
5	J	92	G	C5-C6-O6	-9.36	122.99	128.60
5	I	59	U	O5'-P-OP2	-9.32	97.31	105.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	725	0	362	40	0
1	E	685	0	342	44	0
2	B	10732	0	10828	517	1
2	F	10695	0	10736	702	0
3	C	521	0	299	19	0
3	G	521	0	299	20	0
4	D	225	0	129	3	0
4	H	225	0	129	10	0
5	I	1348	0	678	38	0
5	J	1348	0	678	61	0
All	All	27025	0	24480	1373	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 1373 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LEU:CD1	2:F:154:ILE:HG12	1.37	1.54
2:F:142:LEU:HD11	2:F:154:ILE:CG1	1.39	1.51
2:F:142:LEU:CD2	2:F:154:ILE:HD11	1.41	1.48
2:F:142:LEU:CD2	2:F:154:ILE:CD1	1.94	1.45
2:B:1222:LYS:O	2:B:1318:LEU:CD2	1.66	1.42

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:OD1	2:B:541:SER:OG[2_545]	2.07	0.13

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	1308/1368 (96%)	1268 (97%)	36 (3%)	4 (0%)	37 65
2	F	1313/1368 (96%)	1267 (96%)	41 (3%)	5 (0%)	30 59
All	All	2621/2736 (96%)	2535 (97%)	77 (3%)	9 (0%)	37 65

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1042	ILE
2	F	585	ASP
2	F	1011	GLY
2	F	1020	LYS
2	B	1327	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	1170/1225 (96%)	1131 (97%)	39 (3%)	33 59
2	F	1155/1225 (94%)	1093 (95%)	62 (5%)	18 45
All	All	2325/2450 (95%)	2224 (96%)	101 (4%)	25 51

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	384	ASP

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Mol	Chain	Res	Type
2	F	631	MET
2	F	1338	SER
2	F	425	ARG
2	F	532	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	920	GLN
2	F	807	GLN
2	F	178	ASN
2	F	794	GLN
2	F	46	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	11 (33%)	4 (12%)
1	E	32/34 (94%)	11 (34%)	2 (6%)
5	I	62/65 (95%)	19 (30%)	1 (1%)
5	J	62/65 (95%)	18 (29%)	1 (1%)
All	All	189/198 (95%)	59 (31%)	8 (4%)

5 of 59 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	A
1	A	4	A
1	A	6	G
1	A	9	U

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	J	42	A
5	I	42	A
1	E	3	A
1	A	28	A
1	E	27	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	34/34 (100%)	-0.27	0 100 100	18, 45, 134, 169	0
1	E	32/34 (94%)	0.47	1 (3%) 51 44	38, 77, 181, 216	0
2	B	1322/1368 (96%)	0.36	95 (7%) 23 22	14, 71, 195, 218	0
2	F	1327/1368 (97%)	0.72	186 (14%) 7 10	13, 92, 149, 193	0
3	C	26/26 (100%)	-0.20	1 (3%) 44 37	27, 50, 107, 115	0
3	G	26/26 (100%)	-0.03	1 (3%) 44 37	45, 63, 112, 124	0
4	D	11/11 (100%)	0.27	2 (18%) 4 6	41, 53, 134, 168	0
4	H	11/11 (100%)	0.50	1 (9%) 16 17	41, 59, 110, 175	0
5	I	63/65 (96%)	-0.20	1 (1%) 70 62	20, 74, 126, 157	0
5	J	63/65 (96%)	-0.10	3 (4%) 36 32	36, 56, 156, 192	0
All	All	2915/3008 (96%)	0.49	291 (9%) 14 16	13, 77, 168, 218	0

The worst 5 of 291 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	305	ILE	9.6
2	F	1243	GLU	8.9
1	E	34	G	8.6
2	F	362	TYR	7.4
2	B	900	LEU	6.6

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.